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Structural properties of protective diamond-like-carbon thin films grown on multilayer graphene

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Abstract

In spite of the versatility of electronic properties of graphene, its fragility and low resistance to damage and external deformations reduce the practical value of this material for many applications. Coating of graphene with a thin layer of hard amorphous carbon is considered as a viable solution to protect the 2D material against accidental scratches and other external damaging impacts. In this study, we investigate the relationship between the deposition condition and quality of diamond-like-carbon (DLC) on top of multilayer graphene by means of molecular dynamics simulations. Deposition of carbon atoms with 70 eV incident energy at 100 K resulted in the highest content of sp^3-bonded C atoms that amounted to 15.9%. An increase of the number of dangling bonds at the interface between the top graphene layer and the DLC film indicates that increase of the incident energy reduces the adhesion quality of DLC thin film on graphene. Analysis of radial distribution function indicates that sp^3 hybridized carbon atoms tend to grow near already existing sp^3-atoms. This explains why the quality of the DLC structures grown on graphene have generally a lower content of sp^3 C atoms compared to those grown directly on diamond. Ring analysis further shows that a DLC structure grown on the sp^2-rich structures like graphene contains a higher fraction of disordered ring structures.

Keywords: Diamond-like-carbon, Multilayer graphene, Molecular dynamics, Carbon atoms deposition

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1. Introduction

With the rapid development of nanoscience and nanotechnology, carbon nanomaterials, such as fullerenes [1], carbon nanotubes [2] and graphene [3], have gained much attention. Many scientific efforts are dedicated to study the properties and investigate potential applications of these carbon nanomaterials. Amongst these, graphene is the most promising stable 2D material. Moreover, its unique properties such as mechanical resistance [4], electrical [5] and thermal [6] conductivity etc, compared to conventional macro-materials make graphene a promising material in various applications such as gas sensing [7], water purification, [8] and touch screens [9] in the future. However, the attractive properties of graphene can alter severely due to mechanical wearing, scratching [10], or parasitic irradiation in space applications [11, 12]. The damage of graphene in daily used graphene-based appliances and equipments, will surely shorten the serving time of the latter. Thus, it is of great importance to find a compatible durable coating to protect graphene and enhance its resistant ability against external damage.

Diamond-like-carbon (DLC), is reported to be an ideal protective material for nanostructures and is able to enhance mechanical strength of nanomaterials [13–15]. DLC exhibits many desirable properties, such as ultra-high hardness and elastic moduli [16], low friction coefficient [17], transparency in the IR wavelength band [18] and chemical inertness [19]. Moreover, it is highly compatible with graphene structure. DLC coating is already widely used in many applications, e.g. as an antireflection layer for IR optic devices [20] or a protection layer for magnetic storage components [21] and an anticorrosion layer for biocompatible materials [22]. It will be utilized extensively even more in various fields like electronics, aviation, aerospace etc. [23–25]. In addition, some research has been carried out to analyze the protective properties of DLC films coating nanostructure both experimentally [15, 26–31] and by simulations [32–34]. In particular, Ren *et al.* [35] analyzed the effect of experimental conditions such as the combination of incident energy and ambient temperature on the quality of growing DLC film directly on diamond and on nanotubes placed on a diamond substrate, showing that a stable DLC can grow above a nanotube structure. The above-mentioned research shows that it is feasible to grow a DLC protective layer on top of carbon nanostructures. However, it is not entirely clear what defines the

quality of the grown DLC films, in order to predict their protective properties. Unfortunately there are only few reports about the quality of DLC deposited on top of graphene in different conditions. DLC, which is a variety of amorphous carbon, shows diverse properties with a different ratio of sp^2 and sp^3 hybridization [36]. It was seen that the higher sp^3 fraction the DLC has, the harder and denser it becomes [37]. Therefore, in the current paper we aim to find out how the deposition condition during the growth of thin films can define the quality of DLC above graphene, in order to enable the growth of high quality DLC protective layers.

Atomistic simulation methods are powerful tools to study mechanisms of atomic migration and collision, and eventually, the formation of the bonds within the materials. In this paper, we utilized classical molecular dynamics (MD) to simulate and study the process of carbon ion beam deposition with different incident energies at different temperatures on the top of multilayer graphene. Then, we analyzed the atomic structure, density and sp^3 fraction of grown DLC films in different conditions in order to reveal what inherent mechanisms lead to failure of growth of stable and dense DLC structures.

2. Simulation and analysis methods

Simulations of DLC deposition process shown in this paper were carried out with classical MD code PARCAS [38, 39]. In order to describe the interaction between carbon atoms, the empirical analytical bond-order Brenner-Beardmore potential [40–42] was applied. We used the extended low-end (R=1.95 Å) and high-end (S=2.25 Å) cutoff parameters, following Jäger and Albe's work [43] to improve the description of formation of sp^3-hybridization of carbon atoms. The extended cutoffs allowed depositing DLC with higher sp^3 fraction, which compares better to experimentally grown DLC films [35]. (COMMENT: Kai, could you write up this part with the potentials?) *Unfortunately none of the classical potentials are able to predict correctly the formation of sp^3 bonded atoms [44], however, the selected potential with the extended cutoff can provide the understanding of comparative effect of DLC growth conditions.* All the visualized simulation cells in this paper were obtained with the help of open visualization tool OVITO [45].

Figure 1 shows the schematic diagram of the initial multilayer graphene placed on top of the diamond substrate. For the sake of convenience, all sp^3-hybridized C atoms are colored red in this and the following figures, while sp^2-hybridized C atoms are colored blue. This structure was built up as

follows. The diamond substrate with the $< 111 >$ surface normal and the size of 30×30×20 Åincluded 3456 atoms. Six layers of graphene, 2304 atoms, were placed above the diamond substrate with the layer spacing of 3.35 Å(the interlayer distance in graphite), and the distance between diamond surface and bottom graphene was also 3.35 Å. To minimize the energy of multilayer graphene system, all the six layers of graphene were stacked in the A-B Bernal order. Third, periodic boundary condition was set in lateral (x and y) directions, leaving z-direction an open surface to deposit DLC.

We used the Berendsen [46] thermostat to control the temperature at the lateral borders within the 5 Å region and the two bottom layers of diamond atoms were fixed in order to dissipate heat and prevent the entire system from moving downwards during the continuous carbon ion beam irradiation. At last, incident carbon atoms were set 5 Å above the top layer of graphene with the velocity directed perpendicular to the graphene layers in the direction of the surface. The incident energies for the deposition process was varied between 50, 70, and 100 eV, in different sets of the subsequent deposition simulations. Before each carbon atom impact, a random cell shift in the xy plane was performed to ensure that carbon atoms would hit the whole graphene layer uniformly. Each ion impact was simulated for the total time of 10 ps to allow the generated heat to dissipate naturally at the boundaries of the simulation cell. As carbon atoms were arriving on graphene, the DLC film was gradually growing up and the initial incident position of depositing carbon atoms was also shifted up to ensure that there is always 5 Å distance to the highest z-coordinate of an atom in the cell of the current size to avoid extreme repulsive forces caused due to inappropriately short distances between newly appeared incident atom and already existed DLC. The ambient temperature was set as 100 K during the DLC film deposition. For each energy, around 8000 carbon impacts were carried out to obtain the desired volume of DLC for further analysis.

To evaluate the quality of the grown DLC film, we analyzed the sp^3 fraction, mass density, radial distribution function (RDF), and primitive rings in all the grown structures. We set the first cutoff length as 1.9 Å, as an average value between the first and the second peaks in the total RDF, respectively, see Figure 3. All the atoms with the three neighbours within the selected cutoff were considered as three-fold carbon atoms, or as the sp^2 hybridized ones, while four-fold atoms are counted as having sp^3 hybridization. Apart from the total RDF for all atoms, we also computed the RDF for only the sp^2 and the sp^3 hybridized atoms to deconvolute the total RDF and ana-

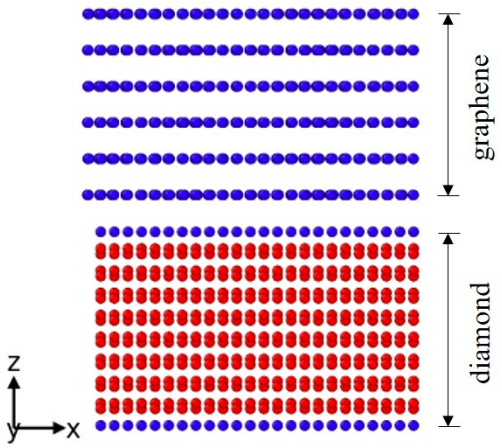

Figure 1: Schematic diagram of diamond and multilayer graphene model. Red atoms represent sp^3 hybridization while blue atoms stand for sp^2 hybridization.

lyze the short range order of both types of atoms in the grown DLC films. To inspect the total disorder degree, we also performed the primitive rings analysis [47]. In addition, the dangling bonds of carbon atoms located in the interface between graphene surface and bottom of the DLC were also analyzed to evaluate adhesion quality of the DLC film.

3. Results and discussion

3.1. sp^3 fraction and mass density

Figure 2 shows the distribution of the sp^3 fraction and mass density of the low-energy-ion deposited DLC film with the different incident energies along the z-axis (perpendicular to the surface) and corresponding simulation cells at 100 K and incident energies of 50, 70, and 100 eV, respectively. The four ticks to the right of the simulation cells are used to guide the eye to the location of the bottom and the top of the simulation cells, as well as of both interfaces (diamond-graphene and graphene-DLC). These four positions corresponds to four turning points in the relevant graphs, see Figure 2(a,c,e). In all these subfigures, the diamond and graphene regions are well visible since diamond has maximum density of 3.6 g/cm^3 and consists of pure sp^3 carbon atoms while graphene has minimum density of 1.8 g/cm^3 and is made of pure sp^2 carbon atoms. As z-coordinate increases, the average density increases fluctuating around 2.7 g/cm^3. At the same time, some increase in

the sp^3 fraction is also observed. This behavior of the mass density and sp^3 fraction indicate the presence of the grown DLC film. We note here that the number of the sp^3-hybridized atoms is slightly higher in the middle of the cell, further away from the interface and the open surface, where excess of the free volume can impede formation of the sp^3-bonds. The stress exerted on sp^2 carbon atoms by deposition of energetic carbon atoms and the continuously growing DLC film, the π C–C bond breaks converting into a σ C–C bond. This process results in formation of four σ covalent bonds corresponding to sp^3 hybridization instead of three σ and one π bonds corresponding to the sp^2 hybridization. On the other hand, the abundance of the sp^2-hybridized carbon atoms in graphene, the first layer of the growing film (right above graphene layers) consists mainly of the same sp^2 carbon atoms, constituting the loose amorphous carbon structure at the bottom of the DLC film.

While analyzing the sp^3 fractions in the DLC grown structures with different incident energies, we see that most sp^3 fraction forming in DLC films grown with 70 eV incident energies than other two energies. This indicates that there exists an optimal incident energy to form highest sp^3 fraction. On the other hand, the images in Figure 2 show that with increase of incident energy of deposited C atoms, fewer layers of the graphene remain intact.

Reduction of the number of graphene layers means that graphene is partially consumed by the grown DLC film and some of the sp^2 carbon atoms from the original graphene layers transformed in the sp^3 hybridized atoms. Hence, the average sp^3 fraction obtained in the cell grown at 100 K with the 70 eV incident carbon ions is higher than that of 50 eV. Although higher deposition energy increases the conversion of the activated graphene sp^2 atoms to become part of the DLC film, it also means that the sp^2-to-sp^3 conversion is promoted due to sufficient local stress generated by more energetic ions capable of penetrating deeper into the cell compared to those of 50 eV energy. This effect makes a notable difference only at low temperature like 100 K since low temperature helps it stabilize the local concentration of the stress. Since sp^2 covalent C–C bonds are energetically more favorable [48], any temperature increase (also due to energetic ion impacts) in the disordered structure of amorphous carbon may reduce the local stress, causing spontaneous transition of forming sp^3 C–C bonds into sp^2 C–C bonds, reducing overall the sp^3 fraction.

The mass density of the DLC films grown under different conditions along with the corresponding sp^3 content are listed in Table 1. We note that the simulation process of the film growth is time-consuming, this is why we report

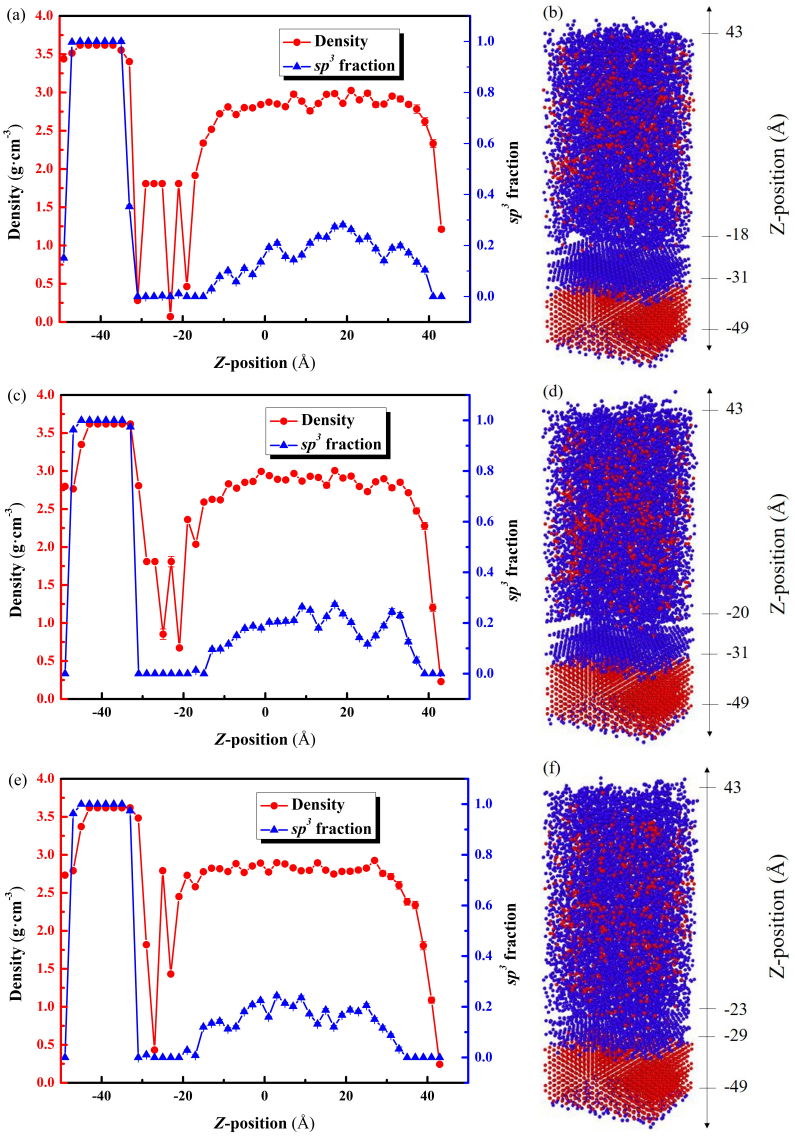

Figure 2: sp^3 fraction (right-hand y-axis) and mass density (left-hand y-axis) of the simulation cells as a function of z-coordinate with the incident energies of a): 50 eV; c): 70 eV; and f) 100 eV. The corresponding post-deposition simulation cells are shown in (b), (d), and (f), respectively. Red circles indicate the atoms with sp^3-hybridized bonds and blue are the atoms with sp^2 ones. The error bars show the standard deviation in the analysis of all the atoms in the corresponding structure.

Table 1: Mass density (g/cm^3) and sp^3 content (%) of DLC films deposited at different incident energies.

Energy (eV)	Mass density (g/cm^3)	sp^3 content (%)
50	2.728	14.9
70	2.766	15.9
100	2.704	13.8

here the results of analysis of a single structure for each energy, aiming mainly qualitative comparison of different deposition conditions. In Figure 2, where the error bars are the standard deviations from the mean value estimated either from the distribution or from the last frames of each of 10 last cascades (incident ion events). In this table, we see that the sp^3 fraction shows much stronger dependence on the incident energy than the average mass density of the grown DLC.

To investigate this effect further we plot now the radial distribution functions for two grown DLC structures with the highest and lowest content of sp^3 atoms to identify the difference in the short range order of all the carbon atoms within this structures. Figure 3 shows the radial distribution function grown with 70 and 100 eV, as well as deconvolution of the peak into the sp^2 and sp^3 components. We show all bonds within the high-end cutoff parameter 2.25 Å of the Brenner potential, which includes only the first nearest neighbors. We see that the expected value of the bond length in the entire structure that was grown at 100 K is around 1.49±0.07 Å and is independent of incident energy. Hereafter the error bars indicate the standard deviation in the value of the bond length for all the atoms in the corresponding structure. For comparison, the bond lengths in graphene and diamond structures in the Brenner interatomic potential with the extended cutoffs used in the present study are 1.459±0.048 Å and 1.545±0.0001 Å , respectively. These values are close to those reported in the experiments, at least for the diamond structure it is known to be 1.54 Å [49]. The bond length in graphene can be estimated as a weighted average between two single bonds and one double bond ($a_{C=C}$ = 1.34 Å [50]), which amounts to 1.47 Å.

When we analyze separately the expected values of the sp^2- and sp^3-bond lengths, we found them to be the same in both structures shown in Figure 3 and amounted to 1.46±0.04 Å and 1.6±0.09 Å, respectively. We see that the average bond length in the grown DLC structures for the sp^2-bonded

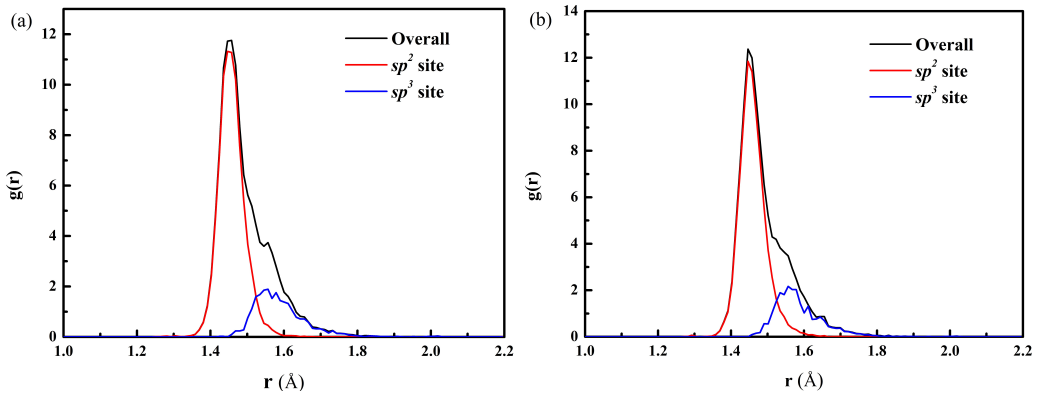

Figure 3: Radial distribution function g(r) for DLC deposited at 100 K under incident energies of (a) 70 and (b) 100 eV, respectively. The contributions of sp^2 and sp^3 coordination are presented separately in red and blue color.

atoms is very close to that in ideal graphene, while the sp^3-bonds are slightly stretched. Also there is some variation in the mean values of the sp^3-bond lengths because of relatively small number of the atoms with such bonds, the amount of these atoms clearly affects the average bond length in the entire structure.

Overall, in both cases we observe much higher peak of the sp^2-bonds compared to sp^3 ones as seen in Figure 3, even for the best structures with the highest density and highest sp^3-content. As it was shown in [35], sp^3 carbon atoms tend to grow near the atoms which already are sp^3-bonded as in diamond. Since we deposited the DLC film on top of graphene layers, the deposited atoms were landing next to the atoms with the sp^2-bonding, forming the same sp^2-bonds in more preferable manner. In other words, we observe the lack of formation of the sp^3-bonded carbon atoms during the initial stage of film deposition, which is consistent with the observations in [35].

Although the bond length of the sp^2-hybridized atoms is shorter, indeed they form only if there is sufficient free volume in the structure. It is also obvious in the values of the mass densities of the grown DLC structures: The higher the sp^3 content in the grown film, the higher its mass density is. In graphite, this inconsistency is explained by the large interlayer distance, while the interlayer distance in amorphous carbon is ill-defined. This is why we further analyze the average atomic volume in the DLC structures with the highest and the lowest sp^3 fraction. For this purpose we employ the

Table 2: Average atomic volume with the standard deviation calculated for the carbon atoms in the DLC films deposited at different temperatures and incident energies.

Energy	Average atomic volume (Å^3)	
(eV)	sp^2 atoms	sp^3 atoms
50	7.53±1.59	6.08±0.65
70	7.44±1.12	6.12±0.66
100	7.58±1.31	6.15±0.61

Voronoi tessellation analysis available in OVITO software. According to this analysis, the average atomic volumes in multilayer graphene and diamond are 9.233±0.345 Å^3 and 5.678±0.001 Å^3, respectively.

In Table 2, we list the average atomic volume separately for sp^2 and sp^3 atoms in DLC films deposited at different incident energies at 100 K. We see that the average atomic volume is larger in the cells with the lowest content of sp^3 bonding, which explains the lower mass density. It is surprising that the atomic volume for the sp^3-bonded atoms is very similar in all structures although it is slightly larger than in pure diamond. This indicates that the formed sp^3 atoms are stable and the bond stretching is mainly explained by the large amount of the sp^2-bonded atoms, which occupy much larger volume per atom. The slightly smaller atomic volume for the sp^2-bonded atoms are explained by densification during the impact.

3.2. Ring analysis

Different atomic volumes occupied by the sp^2-bonded atoms indicates that there can be structural differences in the grown films. To investigate the nature of this differences, we performed the analysis of the primitive rings for quantitative investigation of the degree of long range disorder in the deposited DLC films. We chose the same structures as analyzed in Figure 2, namely the films grown at 100 K with all three incident energies. For this analysis we used the method described in Ref. [47], excluding the top 20 Å of the DLC structure.

In Figure 4, we see that the three DLC structures grown at 100 K have similar distributions of the primitive rings. We see mainly the seven- to ten-member rings, although the number of the six-member rings is only slightly smaller than the larger rings. The five-member rings quite prominent in these structures as well. We see that the amount of the primitive rings with the large number members starts decreasing above 8-member rings in

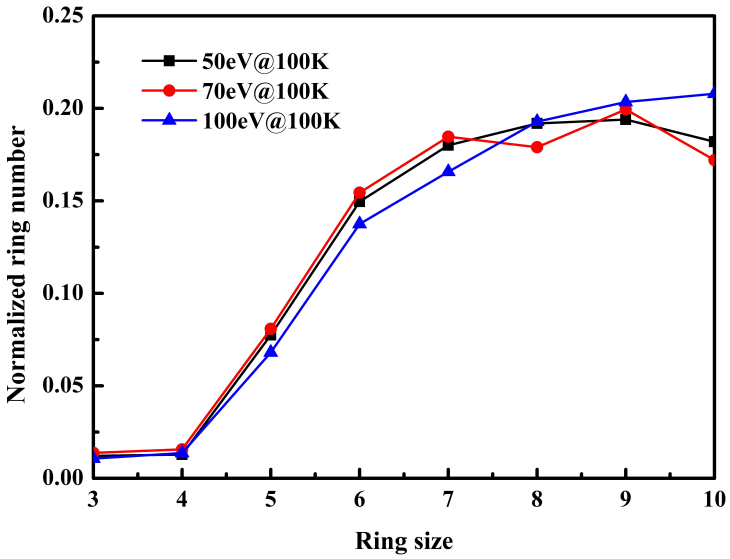

Figure 4: Normalized ring number as a function of ring size at 100 K under 50, 70, and 100 eV, respectively.

the more successful films with the larger quantity of the sp^3 atoms, while the film grown with the 100 eV incident energy exhibits the presence of the primitive rings with the higher number of ten-member rings, which indicates the reduction of structural quality of the film. Compared to the structure of the disordered amorphous carbon rather than graphite indicating that they are quite disordered since the six-element ring represents the structure more close to diamond and is the prefect primitive ring structure. This could be attributed to the relatively low sp^3 fraction in Table 1 compared to Ref. [35]. Even so, DLC generated under 100 eV shows more disordered structure than that under 50 and 70 eV due to the relatively low fraction of six-element rings and high fraction of ten-element rings, meaning that 100 eV produced poorer quality of DLC comparing to other two energies when considering previous data and analysis. DLC deposited under 70 eV is only less disordered in a tiny degree than that under 50 eV comparing the six- and other-element rings. Hence, considering the sp^3 fraction, mass density, and disorder degree, we can draw the conclusion that 70 eV incident energy will lead to better quality of DLC deposited by carbon atoms continuously implanting.

3.3. Dangling bonds

The quality of DLC film is defined not only by the high sp^3 fraction and mass density, but also by the strength of adhesion of the film to the graphene top layer. Loose adhesion of the film to the substrate may result in sliding of the film along the graphene surface under external force. Since the C-C covalent bonds are strong and stable, the atoms with less neighbors than three at least will weaken the adhesion ability of the film in general. In Figure 5 we plot the number of atoms with dangling bonds (< 3 neighbors) as a function of the z-coordinate. We also observe clear peaks at the positions corresponding to the interfaces between diamond and graphene, graphene and DLC, and at the open surface of DLC film. Unsaturated dangling bonds increase the energy of the interface reducing the barrier needed to detach the DLC film from the graphene surface.

Since we are interested in the interface between graphene and DLC, in this study we focus on the second peak from the left in Figure 5. Different symbols in the same plot show the results obtained at 100 K with different incident energies. In Figure 5, there are slightly less atoms with dangling bonds created by ions with 100 eV than with 70 eV and the largest number of the dangling bonds is observed for the lowest incident energy. This clearly indicates that the high incident energy decreases the number of dangling bonds due to more intensive displacement cascades and activated atoms, which helps energetic atoms at the interface form bonds with others. The analysis of the content of dangling bonds in the graphene-DLC interface shows a clear competition between the thermal and radiation-induced processes. In this study, ambient temperature (100 K) is quite low. Therefore, the thermal velocities are very small and the atoms do not have opportunity to saturate the dangling bonds without additional energy introduced by an impacting ion.

Based on this analysis, we conclude that the quality of film adhesion to multilayer graphene increases with increasing incident energy that counterbalanced by the poorer quality of the grown film structure at high energy. This is why, it is important to optimize the film growth condition by carefully selecting the energy of carbon ions during the deposition of the film. Since the peaks for the dangling bonds at this interface created by 70 and 100 eV are almost the same, we conclude that the ions with 70 eV transfer the optimal amount of energy to the lattice atoms to maximize the effect of bond saturation and protect more beneath graphene layers. At lower energy, the transferred energy may not be sufficient and at higher energy induces too

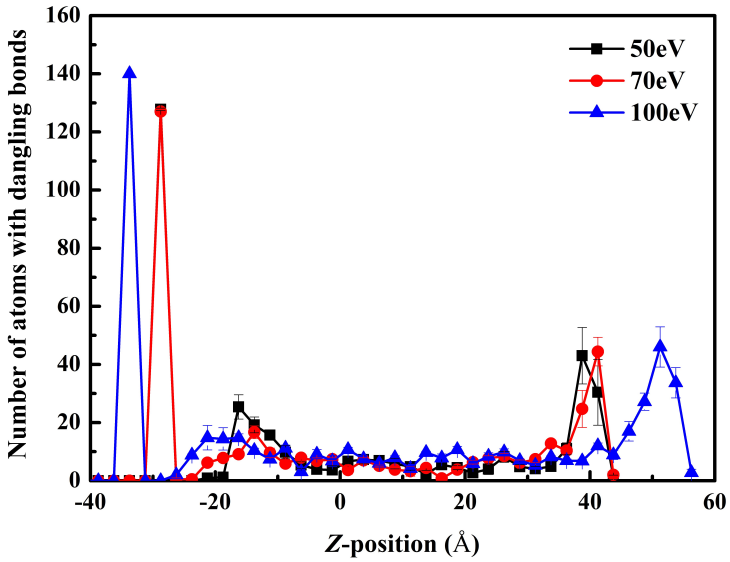

Figure 5: Number of atoms with dangling bonds as a function of z-position under different incident energies at 100 K. Each data point is averaged on the last frame of last 10 incidents and with error bars representing standard deviation.

strong movement of atoms that the bonds remain dangling and also graphene layers are consumed (see the remaining intact graphene layers).

4. Conclusions

In this study, we analyzed the quality of the DLC films deposited on multilayer graphene as a protective layer with different energy of incident carbon ions. We showed that in spite of sp^2-bonding of carbon atoms in graphene, which impedes the formation of sp^3-hybridization, DLC film can grow above graphene by careful selection of optimal deposition condition. We saw that sp^3 hybridization tends to appear in the middle part of DLC along z-direction due to the pressure induced transformation from sp^2 to sp^3 hybridization. Deposition at 70 eV resulted in most fraction of sp^3-bonded atoms and the highest mass density. They dropped with both increasing and decreasing incident energies. In the films, the sp^2-bond length was very close on average to that of graphene, while the sp^3-bond length was slightly longer than that in diamond. Clearly the atomic volume occupied by the sp^2-bonded atoms was much larger than that of sp^3-bonded atoms, but yet, much smaller than in multilayer graphene. By analyzing the primitive rings in the

grown structures, we also concluded that the DLC grows above graphene is mainly disordered structure with a small amount of stable five and six-member rings. At the same time, the quality of the film adhesion improved with increase of incident energy at 100 K. The best adhesion was achieved with the energy of 100 eV. After comprehensive consideration of various situations, we concluded that 70 eV incident energy can provide best quality of DLC film while it can also retain good adhesion ability with graphene layers.

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